

STOICHIOMETRY MEASUREMENTS FOR THE PARAMETERIZATION OF ABSOLUTE RATE MODELS FOR CYTOCHROME P450 METABOLISM

ABSTRACT OF THE DISCLOSURE

5 Systems and method are provided for modeling substrate molecules so that the
various pathway reaction rates, and thus their overall reaction rates and metabolic
properties, can be predicted. The current invention provides various systems and
methods for stoichiometrically measuring the pathway reaction rates, both directly and
indirectly. By repeating this for a class or several classes of substrate molecules, a
10 general model of pathway reaction rates can be developed by correlating observed
pathway reaction rates to the actual structural descriptors of the molecules, in particular,
features around the reactive sites. The model can then be used to predict and design
substrates according to desired metabolic characteristics. The systems and methods are
particularly applicable to metabolism of substrate molecules by the cytochrome P450
15 enzymes.